

Q-CHEM

Fast, Accurate, Robust
Molecular Modeling

Part of the Q-CHEM Suite

COACH Functional

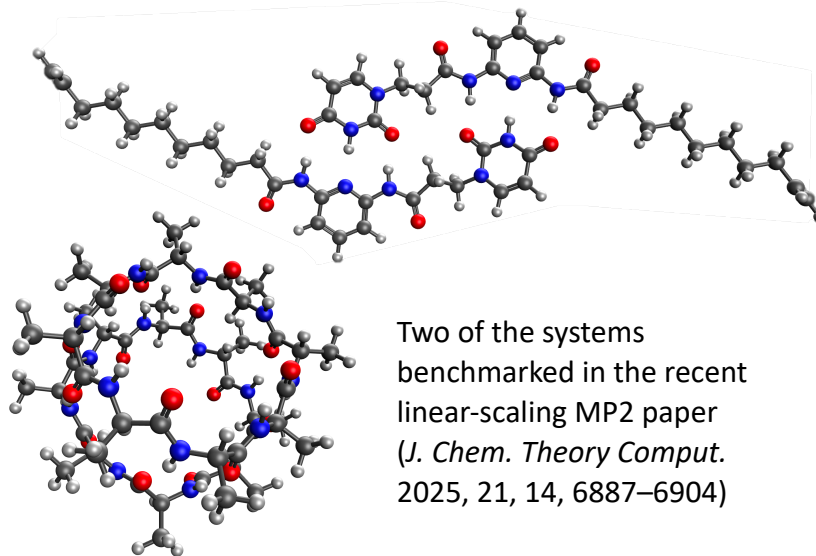
COACH is a new range-separated hybrid (RSH) meta-GGA functional that is more accurate and generally transferable than the best existing RSH meta-GGAs, such as ω B97M-V.

Linear Scaling via Local Correlation

Q-Chem 7 includes a new linear-scaling local correlation algorithm for MP2 and double-hybrid DFT! It is faster and more accurate than DLPNO, and it uses a single numerical threshold, making it easy to tune accuracy.

More Cutting-Edge DFT Features

- Ongoing performance improvements, including RI speedup and MPI
- “Robust SCF” for improved convergence
- New complex-variable functionals
- Complex absorbing potentials (CAP-DFT)



Two of the systems benchmarked in the recent linear-scaling MP2 paper (*J. Chem. Theory Comput.* 2025, 21, 14, 6887–6904)

Black-Box “Robust SCF” Procedure

More robust SCF and DFT convergence, including automatic detection and correction of incipient SCF divergence and algorithm switching. This approach will be valuable in big-data applications and will assist with difficult-to-converge cases.

MRSF-TDDFT

Mixed reference spin-flip TDDFT including energies, properties with SOC, and wavefunction analysis.

New Analysis Tools

A new charge-transfer metric for TDDFT in libwfa. These metrics are rigorously invariant with respect to orbital rotations, unlike earlier metrics such as Tozer’s Lambda, and metrics widely used in the Gaussian program.

Energy decomposition analysis (EDA) can be used to decompose the energy into physically-meaningful components, and now includes ROKS-EDA, EDA OVOCV analysis, and force decomposition analysis (FDA).

New Spectroscopy Tools

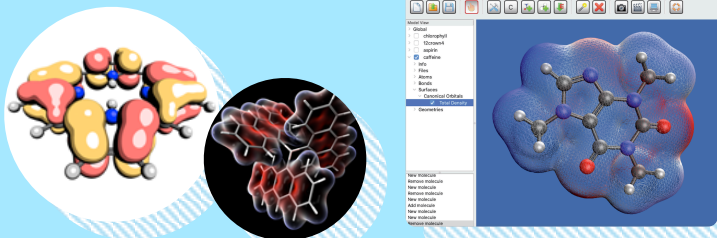
- Restricted and unrestricted VCD
- CVS-XCIS for X-ray spectroscopy modeling
- New methods for modeling Auger decay
- New Δ SCF driver with easy-to-use input and useful analysis and visualization tools

Try Q-Chem

IQmol

IQmol is Q-Chem’s free, open-source molecular editor and visualization package. Use our server to run short Q-Chem jobs!

<https://www.iqmol.org>

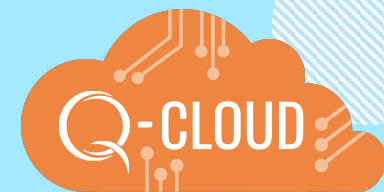


Q-Cloud

No hardware? No problem! Use Q-Cloud to easily run calculations on AWS servers in the cloud.

Free Demo

Request a free demo license, no strings attached!
<https://www.q-chem.com/try>



Q-Chem Open Teamware Project

Q-Chem is a comprehensive suite for molecular, solid state, and biomolecular simulations.



Visit our website!
www.q-chem.com

Density Functional Theory

Q-Chem has a vast built-in library of density functionals. DFT is faster than ever, with great parallel performance and new local correlation methods! Also, try our “Robust SCF” algorithm to easily converge tricky cases.

Solvation, QM/MM, and Embedding

Implicit solvent models, including SMD, C-PCM, and COSMO, explicit solvent modeling, density embedding methods, and QM/MM interfaces to Amber, CHARMM, and GROMACS.

Excited States & Properties

CIS, TDDFT, and EOM-CC and ADC methods.

Post-HF Methods

- Coupled-cluster and algebraic diagrammatic approaches
- RI-CC2
- Local correlation for MP2
- CASSCF, selected CI, and RAS-CI
- Spin-flip (including MRSF-TDDFT)
- Variational 2-RDM

Spectroscopy Modeling

- IR and UV-Vis spectroscopy
- Vibronic spectroscopy
- Photoelectron spectroscopy
- VCD and ECD spectroscopy
- NMR spectroscopy
- Non-linear spectroscopy
- Tools for X-ray spectroscopy: XPS, XAS, XES, Auger, RIXS, and more

Ready-To-Launch Cloud Capabilities

Q-Cloud provides fast and easy cloud computing through Amazon EC2, providing flexibility, scalability, and efficient performance for effective workflows.



Learning & Teaching Resources

Free teaching resources, including lab assignments, video tutorials, webinars, workshops, and lectures.

<https://www.q-chem.com/learn/>



Webinar Series

Hear from experts about the exciting work they're doing in Q-Chem!

<https://www.q-chem.com/webinars/>



Q-Chem Talk Forum

Talk with other users, get help, and review an archive of questions and answers.

<https://talk.q-chem.com/>



Q-Chem Manual

Learn more about features and the underlying theory.

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